

# Metal-Insulator Transition Accompanied with a Charge Ordering in the One-dimensional $t - J'$ Model

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We study the metal-insulator transition accompanied with a charge ordering in the one-dimensional (1D)  $t - J'$  model at quarter filling by the density matrix renormalization group method. In this model the nearest-neighbor hopping energy  $t$  competes with the next-nearest-neighbor exchange energy  $J'$ . We have found that a metal-insulator transition occurs at a finite value of  $t/J'$ ;  $(t/J')_C \simeq 0.18$  and the transition is of first order. In the insulating phase for small  $t/J'$ , there is an alternating charge ordering and the system behaves as a 1D quantum Heisenberg antiferromagnet. The metallic side belongs to the universality class of the Tomonaga-Luttinger liquids. The quantum phase transition is an example of melting of the 1D quantum Heisenberg antiferromagnet.

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Recently low-dimensional copper oxides have attracted much attention as a route to understand the physics of the high- $T_C$  superconductivity. Since the superconductivity in a doped ladder system with a spin gap was theoretically suggested [1], several experimental studies of the quasi one-dimensional (1D) systems with the ladder structure have been carried out. Especially, the discovery of superconductivity in the quasi 1D material  $\text{Sr}_x\text{Ca}_{14-x}\text{Cu}_{24}\text{O}_{41.84}$  ( $x = 0.4$ ) under a high pressure has received considerable interest [2]. The parent material  $\text{Sr}_{14}\text{Cu}_{24}\text{O}_{41}$  includes  $\text{CuO}_2$ -chain layers and  $\text{Cu}_2\text{O}_3$ -ladder layers separated by the Sr layers [3]. Spin excitation gaps are observed in both chains and ladders in ambient pressure [4–6]. The origin of the spin gap in the chain is still controversial in spite of intensive studies [6–11]. By neutron scattering measurements, Matsuda *et al.* concluded [7] that the spin gap in the chain originates from dimer formation between the copper pairs separated by two and four distances of the nearest neighbor copper ions. On the other hand, in more recent neutron scattering measurements [10], Eccleston *et al.* suggested that dimers are formed between next-nearest-neighbor Cu ions which are arranged with a period of 5 Cu-Cu distances in the chain [11]. In the both models considered by Eccleston *et al.* and Matsuda *et al.*, the superexchange interactions between the next-nearest-neighbor Cu spins play an important role.

Matsuda *et al.*'s results have been interpreted in [9] that there exists the alternating  $\text{Cu}^{+2}$  and  $\text{Cu}^{+3}$  order along the chain. According to this scenario, the mean valence of Cu ion in the chain is  $\text{Cu}^{+2.5}$ . On the contrary,  $\text{Cu}^{+2.6}$  is assumed in Eccleston *et al.*'s results [12]. Which scenario is realized is still an open problem. Note that for either case of  $\text{Cu}^{+2.5}$  or  $\text{Cu}^{+2.6}$ , the Cu 3d band is partially filled; the highest 3d band is nearly quarter-filled. Although the Cu 3d band is partially filled, the electrical resistivity of the system shows a semiconducting temperature dependence [4]. Precise understanding

of the semiconducting temperature dependence depends on whether the system is just at the quarter filling or not, since localization effects should be taken into account for the latter case.

In the edge-sharing  $\text{CuO}_2$  chain, the superexchange interaction between next-nearest-neighbor Cu spins through Cu-O-O-Cu path is expected to be more important than the nearest-neighbor superexchange interaction, since in the latter case the bond angle of Cu-O-Cu is close to 90 degree. Thus, the model we consider in the present study is the simplest case where the next-nearest-neighbor superexchange interaction competes with the kinetic energy. For the kinetic energy we consider only the nearest-neighbor hoppings, since in the vicinity of the metal-insulator transition of a quarter filled system the nearest-neighbor hoppings are more important than the next-nearest-neighbor hoppings even if the matrix element of the latter processes is bigger than the former. We assume strong Coulomb repulsion between the  $d$ -electrons, leading to suppression of the double occupancy of the carriers. This model may be called as the one-dimensional  $t - J'$  model where  $t$  represents the nearest-neighbor hoppings and  $J'$  the next-nearest-neighbor exchange.

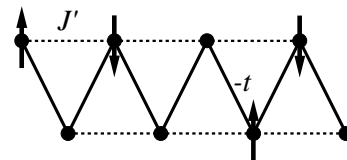


FIG. 1. The  $t - J'$  chain model. Each dot denotes a site and arrows represent carriers with spins specified by arrows.

The model Hamiltonian is defined as

$$\mathcal{H} = -t \sum_{i\sigma} (\tilde{c}_{i\sigma}^\dagger \tilde{c}_{i+1\sigma} + \text{H.c.}) + J' \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+2}, \quad (1)$$

where the operator  $\tilde{c}_{i\sigma}^\dagger$  ( $\tilde{c}_{i\sigma}$ ) creates (annihilates) a particle with a spin  $\sigma$  at  $i$ th site. These operators are defined in the subspace where double occupancy is excluded.  $\mathbf{S}_i$  denotes the spin operator at  $i$ th site. The model is topologically equivalent to the zigzag chain which is shown in Fig. 1. The solid and broken lines denote the nearest-neighbor hoppings  $t$  and the next-nearest-neighbor exchange interactions  $J'$ , respectively.

In this paper we restrict ourselves to the quarter filling. At this filling, the system has two simple limits. (i)  $t \rightarrow 0$ ,  $J'$  is finite : In this limit, all particles localize at odd or even sites, and the system has a gap in the charge excitations. This charge-ordered state behaves as an antiferromagnetic (AF) Heisenberg chain with the exchange interaction  $J'$  [14]. In the AF Heisenberg chain, it is well known that there is no gap in the spin excitations. (ii)  $J' \rightarrow 0$ ,  $t$  is finite : In the case of  $J' = 0$ , the system is identical to the spinless fermions with the macroscopic spin degeneracy of  $2^N$  ( $N$  is the number of spins). For an infinitesimal  $J'$  the spin degeneracy is lifted and the system is expected to belong to the universality class of the Tomonaga-Luttinger (TL) liquids [13]. In this limit, the system is gapless in both the charge and spin excitations. Since the present system has the two limits mentioned above, one can expect that a quantum phase transition occurs at some critical value  $(t/J')_C$  from an insulating phase (the charge gap  $\Delta_c$  is finite) to a metallic phase ( $\Delta_c = 0$ ) as increasing  $t/J'$  from 0 to  $\infty$ . Since particles are expected to order alternatively for a smaller  $t/J'$  than  $(t/J')_C$ , the quantum phase transition is a charge ordering transition.

The purpose of the present study is to answer the following two questions: (i) Does the quantum phase transition occur at a finite  $(t/J')_C$  or already at infinitesimal  $t/J'$ ? (ii) What is the nature of the phase transition? Is it a first- or second-order transition?

In order to determine the transition point, we calculate two quantities: the charge density order parameter  $n_{cd}$  and the charge gap  $\Delta_c$ . In the insulating phase, it is expected that the all particles localize at even or odd sites. Therefore, we consider as the order parameter  $n_{cd} = n_{\text{odd}} - n_{\text{even}}$ , where  $n_{\text{odd}}$  ( $n_{\text{even}}$ ) is the mean value of the number density  $n_i$  at odd (even) sites. The order parameter  $n_{cd}$  is defined as

$$n_{cd} \equiv \frac{1}{L/2} \sum_{i=\text{odd}} (n_i - n_{i+1}). \quad (2)$$

While  $n_{cd}$  should be zero in the metallic phase, it should be finite in the insulating phase. In a finite-size system, the symmetry breaking does not occur if there is no external field. Thus, we calculate  $n_{cd}$  with a small external field  $\epsilon$  at the end of the system. This external field is added to the model Hamiltonian (1) as  $\mathcal{H} - \epsilon \sum_{\sigma} \tilde{c}_{1\sigma}^\dagger \tilde{c}_{1\sigma}$  at the first site ( $\epsilon > 0$ ). We study the response of the system against the small external field.

The charge gap is defined by

$$2\Delta_c(L) \equiv E_g(N_0 + 2, 0; L) + E_g(N_0 - 2, 0; L)$$

$$-2E_g(N_0, 0; L), \quad (3)$$

where  $E_g(N, S_z; L)$  denotes the ground state energy of the system in which the number of particles, the  $z$  component of the total spin and the system size are denoted by  $N$ ,  $S_z$  and  $L$ , respectively. In the quarter-filled case,  $N = N_0 \equiv L/2$ .

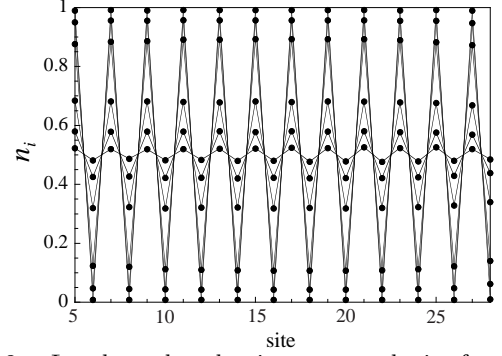


FIG. 2. Local number density  $n_i$  at each site for various values of  $t/J'$ ;  $t/J' = 0.05, 0.10, 0.13, 0.14, 0.15$  and  $0.17$ . For a small  $t/J'$ ,  $n_{\text{odd}} \simeq 1$  and  $n_{\text{even}} \simeq 0$ . This system size  $L$  of this example is 32 ( $\epsilon/J' = 1.0 \times 10^{-3}$ ).

To study the quantum phase transition numerically, it is essential to look at the size dependence systematically and therefore we need to treat large-size systems. To this end, we use the density matrix renormalization group (DMRG) method [15], which is one of the standard numerical methods to study one-dimensional quantum systems. We study systems of various sizes ( $L = 12, 16, 24, 32$ , and  $48$ ) by using the finite-system algorithm of the DMRG method [15]. We keep  $100 \sim 150$  states in the renormalization procedures so that truncation errors in the density matrix are less than  $1.0 \times 10^{-4}$  (typical numerical errors are about  $1.0 \times 10^{-5}$ ).

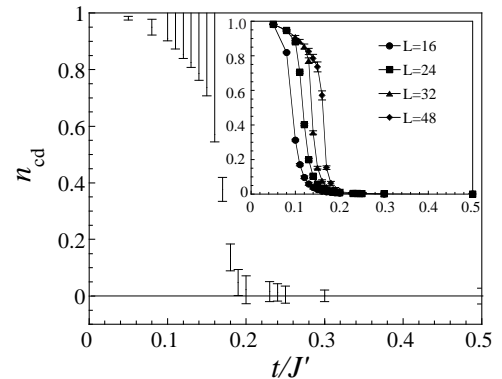


FIG. 3. Results of size extrapolation of  $n_{cd}$  vs  $t/J'$  (see the text). In the inset we plot  $n_{cd}$  for various system sizes.

Figure 2 shows examples of the local number density  $n_i$  for various values of  $t/J'$  with an external field  $\epsilon/J' = 1.0 \times 10^{-3}$  ( $L = 32$ ). Shown here are central 28 sites

excluding 4 sites at both ends of the system. For small  $t/J' (\ll 1)$ , one can clearly see charge ordering behaviors. Most particles spontaneously localize at odd or even sites and in this example the odd sites are selected by the small symmetry breaking field at the first site. For a small  $t/J'$  charge fluctuations are small, i.e.,  $n_{\text{odd}} \simeq 1$  and  $n_{\text{even}} \simeq 0$ . As increasing the value of  $t/J'$ , the difference between  $n_{\text{odd}}$  and  $n_{\text{even}}$  decreases for a fixed system size. Both  $n_{\text{odd}}$  and  $n_{\text{even}}$  approach the mean value of the number density  $N_0/L = 0.5$  for large  $t/J'$ .

Charge density order parameters  $n_{\text{cd}}$  are shown in the inset of Fig. 3 for various system sizes ( $L = 16, 24, 32$ , and  $48$ ). Error bars in the inset represent the standard deviation,

$$\sqrt{\frac{1}{L/2} \sum_{i=\text{odd}} (n_i - n_{i+1})^2 - n_{\text{cd}}^2}, \quad (4)$$

but for most of data they are smaller than the symbols. One can see that as the system size is increased, the disappearance of  $n_{\text{cd}}$  becomes sharper. The region of the charge ordered phase spreads out for larger-size systems. On the other hand, for all system sizes  $n_{\text{cd}}$  vanishes in the region  $t/J' \gtrsim 0.2$ . These results may be an indication that the charge ordering transition is of the first order. However to draw a definite conclusion careful finite size scaling is necessary. Results of size extrapolation of  $n_{\text{cd}}$  are shown in the main part of Fig. 3. We have carried out the linear extrapolation using data for the system size  $L = 24$  and  $32$ . For the transition region  $0.13 \leq t/J' \leq 0.20$ , we have used data for  $L = 32$  and  $48$ . In the case that the extrapolated value obtained by the simple linear extrapolation is greater than 1, the upper error bar is fixed to unity. The values of  $n_{\text{cd}}$  for  $t/J' \gtrsim 0.2$  are extrapolated to zero, while the values below  $t/J' \simeq 0.2$  tend to be finite. Concerning the symmetry breaking field, we have confirmed that  $n_{\text{cd}}$  in the metallic side are suppressed even more and the disappearance of  $n_{\text{cd}}$  becomes sharper for a smaller external field  $\epsilon$  ( $= 1.0 \times 10^{-4} J'$ ).

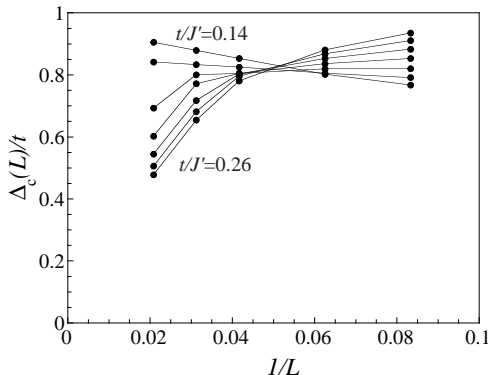


FIG. 4. Size dependence of the charge gap  $\Delta_c(L)$  scaled by  $t$  for several values of  $t/J'$ ;  $t/J' = 0.14, 0.16, 0.18, 0.20, 0.22, 0.24$  and  $0.26$ . Note that the system size dependence is qualitatively different between  $t/J' = 0.14, 0.16$  and  $t/J' \geq 0.18$ .

Now we turn to the charge gap. In Fig. 4, we present the system-size dependence of the charge gap scaled by  $t$  for several values of  $t/J'$ . The system-size dependence of  $\Delta_c(L)$  for  $t/J' \leq 0.16$  is clearly different from that for  $t/J' \geq 0.18$ . For  $t/J' \leq 0.16$ ,  $\Delta_c(L)$  increases as  $L$  is increased, which suggests that the infinite-size limit of  $\Delta_c$  is finite. One can conclude that the system is in the insulating phase for  $t/J' \leq 0.16$ . On the other hand, for  $t/J' \geq 0.18$ , it tends to zero in the infinite-size limit; the system is in the metallic phase. The observed behaviors of the charge gap and the system-size dependence of the charge density order parameters are compatible with the first-order phase transition at  $(t/J')_C \sim 0.18$ .

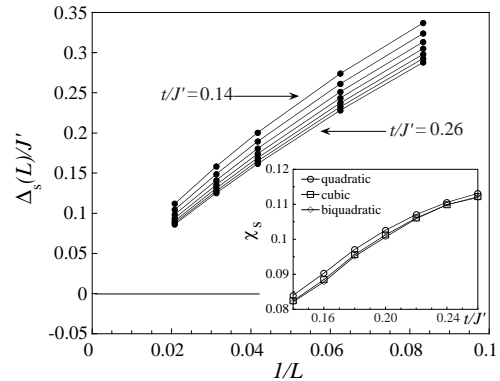


FIG. 5. Size dependence of the spin gap  $\Delta_s(L)$  scaled by  $J'$  for several values of  $t/J'$ ;  $t/J' = 0.14, 0.16, 0.18, 0.20, 0.22, 0.24$  and  $0.26$  (from top to bottom). The inset shows  $\chi_s$  evaluated from  $\Delta_s(L)$  (see the text).

We also calculate the spin gap defined as

$$\Delta_s(L) \equiv E_g(N_0, 1; L) - E_g(N_0, 0; L), \quad (5)$$

in order to see whether there is an anomaly in the spin excitations at the quantum phase transition. The system-size dependence of the spin gap scaled by  $J'$  is shown in Fig. 5. In both (insulating and metallic) phases,  $\Delta_s(L)$  tends to zero in the infinite-size limit and one can conclude that there is no gap in the spin excitations. The slope  $d\Delta_s(L)/d(1/L)|_{(1/L)=0}$  gives the spin susceptibility  $\chi_s$  of the system through the relation  $\Delta_s(L) = 2/(\chi_s L)$  [16]. The coefficient of the linear term is determined by a fitting to a quadratic function including the origin;  $(1/L = 0, \Delta_s(L = \infty) = 0)$ , points for  $L = 48$ ;  $(1/48, \Delta_s(48))$  and for  $L = 32$ ;  $(1/32, \Delta_s(32))$ . We obtain the coefficients also by using cubic and biquadratic functions including four (the origin, points for  $L = 48, 32$ , and  $24$ ) and five (the origin, points for  $L = 48, 32, 24$ , and  $16$ ) points, respectively. The inset of Fig. 5 shows  $\chi_s$  vs  $t/J'$  obtained by the above-mentioned procedures. Good coincidence between the results evaluated from cubic and biquadratic functions indicates that the values thus obtained for  $\chi_s$  are reliable. One can see that  $t/J'$ -dependence of  $\chi_s$  for  $t/J' < 0.18$  may be slightly different from that for  $t/J' \geq 0.18$ , although it

is not possible to conclude whether there is a discontinuity at  $(t/J')_C \simeq 0.18$  or not. Since the phase transition occurs at  $J'$  which is about five times bigger than  $t$ , it is natural to assume that the energy scale of system in the region near the critical point is dominated by  $J'$ . A natural consequence is that the anomaly at the critical point, if any, should be small.

The present model is simple but rather special in the sense that the nearest-neighbor exchange energy  $J$  and the next-nearest-neighbor hopping energy  $t'$  are neglected when  $t$  and  $J'$  are considered. In spite of the special nature of the model, the metal-insulator transition with the charge ordering is generic. To show this, we investigate a few cases with the nearest-neighbor exchange or the next-nearest-neighbor hopping. In Fig. 6, we show  $n_{cd}$  in the following two cases: with an additional nearest-neighbor (ferromagnetic) exchange  $J/J' = -0.5$  and with a next-nearest-neighbor hopping  $t' = t$ . In both cases, for small  $t/J'$ ,  $n_{cd}$  is nearly equal to 1, and it disappears rapidly around some critical value of  $t/J'$ . These behaviors are qualitatively similar to that of the  $t - J'$  chain model which we have discussed in the present paper in detail. In the case with  $J$  ( $t - J - J'$  model), the critical value of  $t/J'$  shifts to a larger value than that of the  $t - J'$  chain model since the hopping energy  $t$  competes with not only  $J'$  but also  $J$ . On the other hand, in the case with  $t' (= t)$  ( $t - t' - J'$  model), the critical value of  $t/J'$  is smaller than that of the  $t - J'$  chain model. This is natural since in the  $t - t' - J'$  model the gain of the kinetic energy in the metallic phase is larger than that in the  $t - J'$  model.

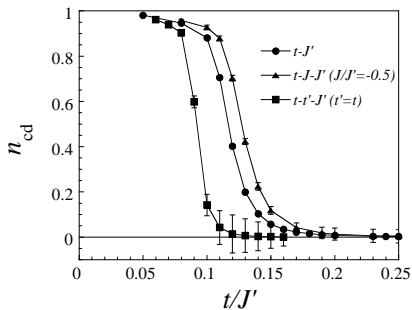


FIG. 6. Comparison of  $n_{cd}$  in the  $t - J - J'$  chain ( $J/J' = -0.5$ ) and  $t - t' - J'$  chain ( $t' = t$ ) with that in the  $t - J'$  chain. The system size is  $L = 32$  ( $\epsilon/J' = 1.0 \times 10^{-3}$ ).

In conclusion, we have calculated the charge density order parameter, the charge gap, and the spin gap obtained in the  $t - J'$  chain model using the DMRG method. We have found that the quantum phase transition from a charge ordered insulator to a metal occurs at  $t/J' \simeq 0.18$  at quarter filling, and the transition is of first order. The transition is generic in the models in which the kinetic energy competes with the next-nearest-neighbor exchange energy at quarter filling. For the present model, an interesting question is existence or absence of the spin gap

close to the metal-insulator transition. The spin excitations are gapless in both limits  $t \rightarrow 0$  and  $J' \rightarrow 0$ . We have found that the spin excitations remain gapless over the whole  $t/J'$  range between the metallic side and the insulating side. The spin susceptibility is obtained from the spin gap of the finite systems. One can see that the  $t/J'$ -dependence of  $\chi_s$  in the metallic phase is slightly different from that in the insulating phase, and there is a possibility that a small anomaly exists at the critical point in the bulk system.

The quantum phase transition discussed in the present paper is an example of melting of the 1D quantum Heisenberg antiferromagnet. In this example, the melting is of first order and the metallic side belongs to the universality class of the TL liquids.

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- [1] E. Dagotto, J. Riera, and D. Scalapino, Phys. Rev. B **45**, 5744 (1992); T. M. Rice, S. Gopalan, and M. Sigrist, Europhys. Lett. **23**, 445 (1993).
  - [2] M. Uehara *et al.*, J. Phys. Soc. Jpn. **65**, 2764 (1996).
  - [3] E. M. McCarron, III *et al.*, Mater. Res. Bull. **23**, 1355 (1988).
  - [4] M. W. McElfresh *et al.*, Phys. Rev. B **40**, 825, (1989).
  - [5] S. A. Carter *et al.*, Phys. Rev. Lett. **77**, 1378 (1996); M. Kato, K. Shiota, and Y. Koike, Physica C **258**, 284 (1996).
  - [6] M. Matsuda and K. Katsumata, Phys. Rev. B **53**, 12201 (1996).
  - [7] M. Matsuda *et al.*, Phys. Rev. B **54**, 12199 (1996).
  - [8] Z. Hiroi *et al.*, Phys. Rev. B **54**, 15849 (1996).
  - [9] N. Motoyama *et al.*, Phys. Rev. B **55**, R3386, (1997).
  - [10] R. S. Eccleston *et al.*, preprint.
  - [11] Very recently, Takigawa *et al.* reported that the result obtained from the NMR measurements is favorable to [10] rather than to [7]: M. Takigawa *et al.*, to appear in Phys. Rev. B.
  - [12] The valence  $\text{Cu}^{+2.6}$  in the chain is simply obtained if one assumes that the valence of Cu in the ladder is  $\text{Cu}^{+2}$ .
  - [13] F. D. M. Haldane, **14**, 2585 (1981).
  - [14] Strictly speaking, in the case of  $t = 0$ , there is the macroscopic degeneracy of configurations of particles in the thermodynamic limit.
  - [15] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10345 (1993).
  - [16] The spin susceptibility  $\chi_s$  is related to the spin velocity  $v_s$  for a TL liquid by the relation  $\chi_s = 1/(2\pi v_s)$ .